Neural Path Features and Neural Path Kernel : Understanding the role of gates in deep learning

Abstract

Rectified linear unit (ReLU) activations can also be thought of as *gates*, which, either pass or stop their pre-activation input when they are *on* (when the pre-activation input is positive) or *off* (when the pre-activation input is negative) respectively. A DNN with ReLU activations has many gates, and the on/off status of each gate changes across input examples as well as network parameters. For a given input example, only a subset of gates are *active*, i.e., on, and the sub-network of weights connected to these active gates is responsible for producing the output. While at randomised initialisation, the active sub-network corresponding to a given input example is random, during training, as the network parameters are learnt, the sub-network is also learnt, and potentially holds very valuable information.

Our aim is to understand the role of the gates, and the dynamics of gate activity during training in DNNs. The gate activity, i.e., the on/off state of the gates of a given input is captured in a novel *neural path feature* (NPF), and the weights of the DNN are encoded in a novel *neural path value* (NPV), and the output of network is expressed as an inner product of NPF and NPV. As a result, the gradient of the output contains two components, each separately responsible for learning the NPFs and NPVs. We show the *neural path kernel* associated with the NPF is a fundamental quantity that characterises the information stored in the gates of a DNN. We show via experiments (on MNIST and CIFAR-10) that in standard DNNs with ReLU activations NPFs are learnt during training and such learning is key for generalisation. Furthermore, NPFs and NPVs can be learnt in two separate networks and such learning also generalises well in experiments. In our experiments, we observe that almost all the information learnt by a DNN with ReLU activations is stored in the gates - a novel observation that underscores the need to further investigate the role of gating in DNNs.

1 Introduction

We consider deep neural networks (DNNs) with rectified linear unit (ReLU) activations. A special property of ReLU activations is that they can also be thought of as *gates*, which are $1/0$ (i.e., on/off) depending on whether or not their pre-activation input is positive or negative. While the weights remain the same across input examples, the $1/0$ state of the gates change across input examples. For each input example, there is a corresponding *active* sub-network consisting of those gates which are 1, and the weights which pass through such gates. This active sub-network can be said to hold the memory for a given input, i.e., only those weights that pass through such active gates contribute to the output. In this viewpoint, at random initialisation of the weights, for a given input example, a random sub-network is active and produces a random output. However, as the weights change during training (say via gradient descent), the $1/0$ states of the gates, and hence the active sub-networks corresponding to the various input examples also change. At the end of training, for each input example, there is a learned active sub-network, and produces the learned output. Thus, the gates could potentially contain valuable information.

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In this paper, our aim is to understand the role of the gates, and the dynamics of gate activity while training DNNs using gradient descent. Our findings can be summarised in the following claims which we theoretically/experimentally justify in the paper:

Claim I: *Information in the gates of a DNN is captured in its active sub-networks.*

Claim II: *Dynamics of the gates, i.e., the changes in the* $1/0$ *states of the gates during training, is key for generalisation.*

Notation: We consider fully-connected DNNs with w hidden units per layer and $d-1$ hidden layers. The DNN accepts an input $x \in \mathbb{R}^{d_{in}}$ and produces an output $\hat{y}_\Theta(x) \in \mathbb{R}$, where $\Theta \in \mathbb{R}^{d_{net}}$ are the network parameters ($d_{net} = d_{in}w + (d-2)w^2 + w$). We denote by $\Theta(l,j,i)$, the weight connecting the j^{th} hidden unit of layer $l-1$ to the i^{th} hidden unit of layer $l \in [d]$. The dataset is given by $(x_s, y_s)_{s=1}^n \in \mathbb{R}^{d_{in}} \times \mathbb{R}$. The loss function is given by $L_\Theta = \frac{1}{2}\sum_{s=1}^n \left(\hat{y}_\Theta(x_s) - y_s\right)^2$. We consider the gradient descent update given by $\Theta_t = \Theta_t - \alpha_t(\nabla_\Theta L_\Theta)$, where $\alpha_t > 0$ is a small step-size and $\nabla_\Theta(\cdot)$ stands for the gradient of $(\cdot)$ with respect to the network parameters. We denote the set $\{1,\ldots,n\}$ by $[n]$. We use vectorised notations: $y = (y_s, s \in [n]), \hat{y}_\Theta = (\hat{y}_\Theta(x_s), s \in [n]) \in \mathbb{R}^n$ for the true and predicted outputs and $e_\Theta = (\hat{y}_\Theta - y) \in \mathbb{R}^n$ for the error in the prediction.

1.1 Background: Neural Tangent Feature and Kernel

The *neural tangent feature and kernel* (NTF and NTK) machinery was developed in some of the recent works [4, 1, 2, 3] related to optimisation and generalisation in DNNs trained using gradient descent. For an input $x \in \mathbb{R}^{d_{in}}$, the NTF is given by $\psi_{x,\Theta} = \nabla_\Theta \hat{y}_\Theta(x) \in \mathbb{R}^{d_{net}}$, i.e., the gradient of the network output with respect to its weights. The NTK matrix on the dataset is the $n \times n$ Gram matrix of the NTFs of the input examples, and is given by $K_\Theta(s,s') = \langle \psi_{x_s,\Theta}, \psi_{x_{s'},\Theta}\rangle, s, s' \in [n]$.

Proposition 1.1 (Lemma 3.1 Arora et al. [2019]**).** *For the infinitesimally small step-size of GD procedure, the dynamics of the error term can be written as* $\dot{e}_t = -K_{\Theta_t} e_t$.

Prior Results(Jacot et al. [2018], Arora et al. [2019], Cao and Gu [2019])**:** Under randomised initialisation, and in the limit of 'large-width', i.e., width w far exceeding the number of data points, an interesting property emerges: the parameters of the DNN deviate very little during training, i.e. $\Theta_t \approx \Theta_0$. In particular, , $K_{\Theta_0} \to K^{(d)}$ as $w \to \infty$, and $K_{\Theta_t} \approx K_{\Theta_0}$, i.e., the NTK matrix at initialisation K_{Θ_0} converges to a deterministic matrix $K^{(d)}$ and stays almost constant through training. In the 'large-width' case, Arora et al. [2019] show that the fully trained DNN is equivalent to kernel regression with $K^{(d)}$. Hence, a trained DNN enjoys the generalisation ability of its corresponding $K^{(d)}$ matrix in the 'large-width' regime. Cao and Gu [2019] show that in the case of 'large-width', the DNN is almost a linear learner with the random NTFs, and showed a generalisation bound in the form of $\tilde{\mathcal{O}}\left(d \cdot \sqrt{y^\top \left(K^{(d)}\right)^{-1} y/n}\right)$[1].

Research Gap: In the 'large-width' case, the research gap is both a *conceptual* as well as that of *performance*. Here, DNNs are linear learners using the random NTFs at random initialisation, and this does not explain feature learning in practical DNNs with finite width; this is a conceptual gap. Arora et al. [2019] noted that, while pure-kernel methods based on the limiting Convolutional NTK (CNTK) outperform other state-of-the-art kernel methods, the finite width CNNs still outperform their CNTK counterpart; this is a performance gap.

1.2 Organisation

In Section 2, we encode the state of the gates in a novel neural path feature (NPF) and the weights in a novel neural path value (NPV), and we express the output of the DNN as an inner product of NPF and NPV. We 'plugin' this inner product expression to expand the NTF and NTK, wherein, we capture the dynamics of the gates via terms related to NPF learning. This addresses the conceptual gap related to feature learning. In Section 4 we introduce a deep gated network (DGN) framework that decouples the NPF and the NPV, as a result of which we have two learning problems namely fixed NPF learning and decoupled NPF learning. In **??**, we derive theory to support Claim I by showing that in the limit of infinite width, the optimisation and generalisation of fixed NPF learning is tied down to the NPK.

[1] $a_t = \mathcal{O}(b_t)$ if $\limsup_{t\to\infty} |a_t/b_t| < \infty$, and $\tilde{\mathcal{O}}(\cdot)$ is used to hide logarithmic factors in $\mathcal{O}(\cdot)$.

In Section 6, we support Claim II experimentally. We show that in finite width DNNs with ReLU activations, NPF learning happens continuously (NPFs at later stages of training are better than NPFs in the initial stages) during training, and such learning is key for generalisation. The highlights are:

• The NPF and NPV are *primitive/fundamental* quantities, in that, they are zeroth-order, and the first-order gradient based quantities namely NTF/NTK can be derived using NPF and NPV.

• The NPK can be decomposed as a *Hadamard* product of the input Gram matrix, and a correlation matrix of active sub-network overlaps. Thus the information stored in the gates/NPFs is *interpretable* in terms of the active sub-networks.

2 Neural Path Feature and Kernel: Encoding Gating Information

First step in understanding the role of gates is to explicitly *encode* the $1/0$ states of the gates. The gating property of the ReLU activation allows us to express the output of the network as a summation of the contribution of the individual paths, and paves a natural way to encode the $1/0$ states of the gates *without loss of information*. The contribution of a path is the product of the signal in its input node, the 'd' weights in the path and the '$(d-1)$' gates in the path. For an input $x \in \mathbb{R}^{d_{in}}$, and parameter $\Theta \in \mathbb{R}^{d_{net}}$, we encode the gating information in a novel *neural path feature* (NPF), $\phi_{x,\Theta} \in \mathbb{R}^P$ and the weights in a novel *neural path value* (NPV) $v_\Theta \in \mathbb{R}^P$, where, $P = d_{in}w^{(d-1)}$ is the total number of paths. The NPF co-ordinate of a path is the product of the signal at its input node and the gates in the path. The NPV co-ordinate of a path is the product of the weights in the paths. This allows us to express the output of the DNN as an inner product of the NPFs and NPVs, i.e., $\hat{y}_\Theta(x) = \langle \phi_{x,\Theta}, v_\Theta \rangle$.

By stacking the NPFs of all the input examples we obtain the NPF matrix as $\Phi_\Theta = (\phi_{x_s,\Theta}, s \in [n]) \in \mathbb{R}^{P\times n}$. Then the input-output relationship of a DNN in vector form is given by:

$$\hat{y}_\Theta = \Phi_\Theta^\top v_\Theta \tag{1}$$

Thus gradient descent on $\Theta \in \mathbb{R}^{d_{net}}$ changes both quantities Φ_Θ and v_Θ, of which, Φ_Θ captures the information in the gates. Further, the NPV is a P dimensional quantity, however, loosely speaking, its 'degrees of freedom' is restricted by its parameter Θ, whose dimension is d_{net}.

The associated *neural path kernel* (NPK) matrix defined as $H_\Theta = \Phi_\Theta^\top \Phi_\Theta$, has a special property, in that, it can be written as the *Hadamard* product of the input Gram matrix Σ, and matrix Λ_Θ which is a correlation matrix of active sub-networks. Note that Σ is a constant, while Λ_Θ is learnt during training.

2.1 Paths

Input Layer	$z_{x,\Theta}(0)$	$=$	x
Pre-Activation	$q_{x,\Theta}(l,i)$	$=$	$\Theta(l,\cdot,i)^\top z_{x,\Theta}(l-1), l \in [d-1], i \in [w]$
Gating Values	$G_{x,\Theta}(l,i)$	$=$	$\gamma(q_{x,\Theta}(l,i)), l \in [d-1], i \in [w]$
Hidden Layer	$z_{x,\Theta}(l,i)$	$=$	$\chi(q_{x,\Theta}(l,i)) = q_{x,\Theta}(l,i) \cdot G_{x,\Theta}(l,i), l \in [d-1], i \in [w]$
Final Output	$\hat{y}_\Theta(x)$	$=$	$\Theta(d)^\top z_{x,\Theta}(d-1)$

Table 1: Here $\Theta(1) \in \mathbb{R}^{w\times d_{in}}, \Theta(l) \in \mathbb{R}^{w\times w}, \forall l \in \{2,\ldots,d-1\}, \Theta(d) \in \mathbb{R}^{w\times 1}$.

A path starts from an input node, passes through exactly one weight (and one hidden node) in each layer and ends at the output node. We have a total of $P = d_{in}w^{(d-1)}$ paths. Let us say that an enumeration of the paths is given by $[P] = \{1,\ldots,P\}$. Let $\mathcal{I}_l \colon [P] \to [w], l = 0,\ldots,d-1$ provide the index of the hidden unit through which a path p passes in layer l (with the convention that $\mathcal{I}_d(p) = 1, \forall p \in [P]$).

2.2 Neural Path Feature, Neural Path Value and Network Output

Definition 2.1. *Let $x \in \mathbb{R}^{d_{in}}$ be the input to the DNN. For this input,*

(i) The activity of a path p is given by : $A_\Theta(x,p) \stackrel{def}{=} \Pi_{l=1}^{d-1} G_{x,\Theta}(l,\mathcal{I}_l(p))$.

(ii) The neural path feature (NPF) is given by : $\phi_{x,\Theta} \stackrel{def}{=} (x(\mathcal{I}_0(p))A_\Theta(x_s, p), p \in [P]) \in \mathbb{R}^P$.

(iii) The neural path value (NPV) if given by : $v_\Theta \stackrel{def}{=} \left(\Pi_{l=1}^d \Theta(l, \mathcal{I}_{l-1}(p), \mathcal{I}_l(p)), p \in [P]\right) \in \mathbb{R}^P$.

In Definition 2.1, for a path p, $\mathcal{I}_0(p)$ is the input node at which the path starts, and $A_\Theta(x,p)$ is its activity. Thus, for a path p, its coordinate $\phi_{x,\Theta}(p)$ is 0 if any one of the gates in the path is off, and is equal to the signal at the input node if all the gates in the path are on. Further, in the case of DNN with ReLU activations, the NPFs are *positively homogeneous*, i.e., $\phi_{cx,\Theta} = c\phi_{x,\Theta}, \forall c > 0, x \in \mathbb{R}^{d_{in}}$.

Proposition 2.1. *The output of the network can be written as an inner product of the NPF and NPV, i.e.,* $\hat{y}_\Theta(x) = \langle \phi_{x,\Theta}, v_\Theta \rangle = \sum_{p\in[P]} x(\mathcal{I}_0(p))A_\Theta(x,p)v_\Theta(p)$.

2.3 Neural Path Kernel: Similarity based on active sub-networks

Definition 2.2. *For input examples* $s, s' \in [n]$ *define*

1. $\tau_\Theta(s, s', l) \stackrel{def}{=} \sum_{i=1}^w G_{x_s,\Theta}(l,i) G_{x_{s'},\Theta}(l,i)$ *be the number of activations that are "on" for both inputs* $s, s' \in [n]$ *in layer* $l \in [d-1]$.

2. $\Lambda_\Theta(s, s') \stackrel{def}{=} \Pi_{l=1}^{d-1} \tau_\Theta(s, s', l)$.

For a given example $s \in [n]$, $\Lambda_\Theta(s,s)$ is a measure of the total number of active paths for that input example, and for different input examples $s, s' \in [n]$ it is a measure of total number of paths that are active for both examples $s, s' \in [n]$. Thus, $\Lambda_\Theta \in \mathbb{R}^{n\times n}$ is the correlation matrix that measures the amount of overlap the active sub-networks.

Lemma 2.1. *Let* $\Sigma \in \mathbb{R}^{n\times n}$ *be the* $n \times n$ *input Gram matrix with* $\Sigma(s,s') = \langle x_s, x_{s'} \rangle, s, s' \in [n]$. *It follows that* $H_\Theta = \Sigma \odot \Lambda_\Theta$*, where* $\odot$ *stands for the Hadamard product.*

3 Neural Path Feature Learning: Dynamics of Gates in Gradient Descent

In Section 2, we encoded the gating information into the NPFs. In this section, we capture the gating dynamics via a NPF learning term denoted by $\dot{\phi}_{x,\Theta_t}$. We achieve this by plugging $\hat{y}_\Theta(x) = \langle \phi_{x,\Theta}, v_\Theta \rangle$ to expand $\psi_{x,\Theta}$ and K_Θ. It is straightforward to note that $\psi_{x,\Theta} = \psi^{\text{V}}_{x,\Theta} + \psi^{\text{F}}_{x,\Theta}$, where $\psi^{\text{V}}_{x,\Theta}$ and $\psi^{\text{F}}_{x,\Theta}$ denote the gradients of the NPV and NPF with respect to the network parameters. Thus, gradient descent can be said to learn both the NPV and the NPF. By carrying out the algebra all the way through K_Θ, we specify the gradient descent dynamics, wherein, gating dynamics is captured by a NPF learning term.

3.1 Expanding Neural Tangent Features and Neural Tangent Kernel

By 'plugging' the expression for $\hat{y}_\Theta(x)$ in $\partial_\theta \hat{y}_\Theta(x)$, we have

$$\begin{aligned}\partial_\theta \hat{y}_\Theta(x) &= \underbrace{\langle \phi_{x,\Theta}, \partial_\theta v_\Theta \rangle}_{\text{value derivative}} + \underbrace{\langle \partial_\theta \phi_{x,\Theta}, v_\Theta \rangle}_{\text{feature derivative}} \\ &= \sum_{p\in[P]} x(\mathcal{I}_0(p))A_\Theta(x,p)\partial_\theta v_\Theta(p) + \sum_{p\in[P]} x(\mathcal{I}_0(p))\partial_\theta A_\Theta(x,p)v_\Theta(p)\end{aligned} \tag{2}$$

Note that due to the $A_\Theta(x,p)$, only active paths (those passing through active gates) contribute to the value derivative, and due to the $\partial A_\Theta(x,p)$, only sensitive paths (those passing through sensitive gates) contribute to the feature derivative. The next two results Propositions 3.1 and 3.2 characterise the $\partial_\theta v_\Theta(p)$ and the $\partial_\theta A_\Theta(x,p)$ terms.

Proposition 3.1. *Let* p *be a path, and let* $\theta \in \Theta$ *be an arbitrary weight belonging to layer* $l' \in [d]$ *such that* $\theta = \Theta(l', i, j)$. *Then* $\partial_\theta v_\Theta(p) = 0$ *if the path does not pass through the weight, and* $\partial_\theta v_\Theta(p) = \Pi_{l\neq l', l=1}^d \Theta(l, \mathcal{I}_{l-1}(p), \mathcal{I}_l(p))$.

Proposition 3.2. *Let* p *be a path, and let* $\theta \in \Theta$ *be an arbitrary weight, then* $\partial_\theta A_\Theta(x,p) = \sum_{l=1}^d \partial G_{x,\Theta}(l) \Pi_{l'\neq l} G_{x,\Theta}(l')$

From (2) we have $\psi_{x,\Theta}=\psi^{\text{V}}_{x,\Theta}+\psi^{\text{F}}_{x,\Theta}$, where ψ^{V} and ψ^{F} denote the value and feature gradients given by $\psi^{\text{V}}_{x,\Theta}=(\langle\phi_{x,\Theta},\partial_\theta v_\Theta\rangle,\theta\in\Theta)\in\mathbb{R}^{d_{net}}$ and $\psi^{\text{F}}_{x,\Theta}=(\langle\partial_\theta\phi_{x,\Theta},v_\Theta\rangle,\theta\in\Theta)\in\mathbb{R}^{d_{net}}$ respectively. The NTK matrix is given by $K_\Theta(s,s')=\langle\psi_{x_s,\Theta},\psi_{x_{s'},\Theta}\rangle$, $s,s'\in[n]$ and can be further decomposed as:

$$K_\Theta(s,s')=\underbrace{K^{\text{V}}_\Theta(s,s')}_{\langle\psi^{\text{V}}_{x_s,\Theta},\psi^{\text{V}}_{x_{s'},\Theta}\rangle}+\underbrace{K^{\text{F}}_\Theta(s,s')}_{\langle\psi^{\text{F}}_{x_s,\Theta},\psi^{\text{F}}_{x_{s'},\Theta}\rangle}+\underbrace{K^{\text{CROSS}}_\Theta(s,s')}_{\langle\psi^{\text{V}}_{x_s,\Theta},\psi^{\text{F}}_{x_{s'},\Theta}\rangle+\langle\psi^{\text{F}}_{x_s,\Theta},\psi^{\text{V}}_{x_{s'},\Theta}\rangle}\tag{3}$$

3.2 Gradient Descent Dynamics in DNN with ReLU

An important point to note here is that the derivative of the ReLU gates (i.e., $1/0$ state) with respect to its pre-activation is almost surely 0. As a result, in (2) $\partial_\theta A_\theta(\cdot,\cdot)=0$ and hence $\psi^{\text{F}}_{x,\Theta}=0$, $K^{\text{F}}_\Theta=K^{\text{CROSS}}_\Theta=0$. However, ϕ_{x,Θ_t} changes at discrete time instants, and the system 'switches' its behaviour.

Definition 3.1. *Define a sequence of monotonically increasing time instants $\{T_i\}_{i=0}^\infty$ (with $T_0=0$) to be 'switching' instants if $\phi_{x_s,\Theta_t}=\phi_{x_s,\Theta_{T_i}},\forall s\in[n],\forall t\in[T_i,T_{i+1}),i=0,\ldots,\infty$, and $\forall i=0,\ldots,\infty\ \exists s(i)\in[n]$ such that $\phi_{x_{s(i)},\Theta_{T_i}}\neq\phi_{x_{s(i)},\Theta_{T_{i+1}}}$.*

The following result describes GD dynamics under such a switching behaviour.

Proposition 3.3. *Let $\nabla_\Theta v_\Theta(p,\theta)=\partial_\theta v_\Theta(p),\forall\theta\in\Theta,p\in[P]$ be a $P\times d_{net}$ matrix of NPV derivatives. Then for $t\in[T_i,T_{i+1})$ and infinitesimally small step-size of GD:*

(i) $\dot{e}_t=-K_{\Theta_t}e_t$, where $K_{\Theta_t}=\Phi^\top_{\Theta_{T_i}}\left((\nabla_\Theta v_{\Theta_t})(\nabla_\Theta v_{\Theta_t})^\top\right)\Phi_{\Theta_{T_i}}$.

(ii) $\rho_{min}(K_{\Theta_t})\leq\rho_{\min}(H_{\Theta_{T_i}})\rho_{\max}\left((\nabla_\Theta v_{\Theta_t})(\nabla_\Theta v_{\Theta_t})^\top\right)$.

Remark: Informally speaking, H_Θ will be ill-conditioned when there exists input examples $s,s'\in[n]$ in the dataset that are almost same, as a consequence of which the s^{th} and ${s'}^{th}$ rows (as well as columns) of the symmetric matrices Σ and Λ_Θ are very close (due to the similarity in active sub-networks for the two inputs that very close). This is quite intuitive, as in, the closer two inputs are, the closer are their NPFs, and it is harder to train the network to produce arbitrarily different outputs for such inputs that are very close to one another.

3.3 Gradient Descent Dynamics With Neural Path Feature Learning

We remedy the non-differentiability of $1/0$ state of the gates by the use of *soft-ReLU* gates, where the gating and activations are given by $\gamma_{sr}(q)=\frac{1}{(1+\exp(-\beta\cdot q))},\beta>0$, and $\chi_{sr}(q)=q\cdot\gamma_{sr}(q)$ respectively. The derivative of soft-ReLU gating with respect to its pre-activation is given by $\partial_q\gamma_{sr}(q)=\frac{\beta}{(1+\exp(\beta\cdot q))(1+\exp(-\beta\cdot q))}$. The soft-ReLU gating is to be regarded as a 'trick' to analytically relax the $1/0$ state and track its change in a continuous manner.

Proposition 3.4. *For small step-size $\alpha_t\to0$, the gradient descent dynamics with NPF learning can be given by:*

Weights	$\dot{\Theta}_t$	$=$	$-\sum_{s=1}^n\psi_{x_s,\Theta_t}e_t(s)=\sum_{s=1}^n(\psi^{\text{V}}_{x_s,\Theta_t}+\psi^{\text{F}}_{x_s,\Theta_t})e_t(s)$
NPF	$\dot{\phi}_{x_s,\Theta_t}(p)$	$=$	$x(\mathcal{I}_0(p))\sum_{\theta\in\Theta}\partial_\theta A_{\Theta_t}(x_s,p)\dot{\theta}_t,\forall p\in[P],s\in[n]$
NPV	$\dot{v}_{\Theta_t}(p)$	$=$	$\sum_{\theta\in\Theta}\partial_\theta v_{\Theta_t}(p)\dot{\theta}_t,\forall p\in[P]$
Error	$\dot{e}_t$	$=$	$-K_{\Theta_t}e_t$, where $K_\Theta=K^{\text{V}}_\Theta+K^{\text{F}}_\Theta+K^{\text{CROSS}}_\Theta$

4 Deep Gated Networks: Decoupling Neural Path Feature and Value

In order to ascertain that NPF learning indeed makes a difference, we should measure the generalisation performance with and without the NPF learning. This can be achieved by a deep gated network (see Figure 1 below for details) having two networks of identical architecture namely i) a feature network parameterised by $\Theta^{\text{F}}\in\mathbb{R}^{d_{net}}$, that holds gating information, and hence the NPFs and ii) a value network that holds the NPVs parameterised by $\Theta^{\text{V}}\in\mathbb{R}^{d_{net}}$. By making $\Theta^{\text{F}}\in\mathbb{R}^{d_{net}}$

trainable/non-trainable, we can *enable/disable* the NPF gradient, which gives rise to the following two modes of operating a DGN:

1. **Fixed NPF (FNPF):** Here, $\Theta^{\text{F}}_t = \Theta^{\text{F}}_0, \forall t \geq 0$, i.e., $\Theta^{\text{F}} \in \mathbb{R}^{d_{net}}$ is non-trainable. Thus the DGN learns the relation $\hat{y}_{\Theta^{\text{DGN}}} = \Phi^{\top}_{\Theta^{\text{F}}_0} v_{\Theta^{\text{V}}}$, where $\Phi_{\Theta^{\text{F}}_0} \in \mathbb{R}^{P\times n}$ is a fixed NPF matrix, and $v_{\Theta^{\text{V}}}$ is learned via gradient descent on $\Theta^{\text{V}} \in \mathbb{R}^{d_{net}}$.

2. **Decoupled NPF Learning (DNPFL):** Here both $\Theta^{\text{F}} \in \mathbb{R}^{d_{net}}$ and $\Theta^{\text{V}} \in \mathbb{R}^{d_{net}}$ are trained, and the DGN learns the relation $\hat{y}_{\Theta^{\text{DGN}}} = \Phi^{\top}_{\Theta^{\text{F}}} v_{\Theta^{\text{V}}}$. In comparison to (1), here we have two parameters $\Theta^{\text{V}} \in \mathbb{R}^{d_{net}}$ and $\Theta^{\text{V}} \in \mathbb{R}^{d_{net}}$ as opposed to a single $\Theta \in \mathbb{R}^{d_{net}}$ in (1).

Note: FNPF and DNPFL are idealised modes to understand the role of gates, and not alternate proposals to replace standard DNNs with ReLU activations.

Layer	Feature Network (NPF)	Value Network (NPV)
Input	$z^{\text{F}}_{x,t}(0) = x$	$z^{\text{V}}_{x,t}(0) = x$
Activation	$q^{\text{F}}_{x,t}(l) = \Theta^{\text{F}}_t(l)^{\top} z^{\text{F}}_{x,t}(l-1)$	$q^{\text{V}}_{x,t}(l) = \Theta^{\text{V}}_t(l)^{\top} z^{\text{V}}_{x,t}(l-1)$
Hidden	$z^{\text{F}}_{x,t}(l) = \chi^{\text{F}}\left(q^{\text{F}}_{x,t}(l)\right)$	$z^{\text{V}}_{x,t}(l) = q^{\text{V}}_{x,t}(l) \odot G_{x,t}(l)$
Output	None	$\hat{y}_t(x) = \Theta^{\text{V}}(d)^{\top} z^{\text{V}}_{x,t}(d-1)$
Gating Values: $G_{x,t}(l) = \gamma_r\left(q^{\text{F}}_{x,t}(l)\right)$ or $G_{x,t}(l) = \gamma_{sr}\left(q^{\text{F}}_{x,t}(l)\right)$		

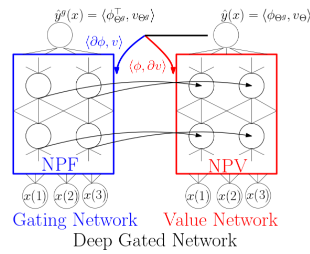

Figure 1: Deep gated network (DGN) setup. The pre-activations $q^{\text{F}}_{x,t}(l)$ of layer $l \in [d-1]$ from the feature network are used to derive the gating values $G_{x,t}(l)$ of layer $l \in [d-1]$.

Proposition 4.1 (DGN)**.** *Let* $\psi^F_{x,\Theta^{DGN}} \stackrel{def}{=} \nabla_{\Theta^F} \hat{y}_{\Theta^{DGN}}(x) \in \mathbb{R}^{d_{net}}$, $\psi^V_{x,\Theta^{DGN}} \stackrel{def}{=} \nabla_{\Theta^V} \hat{y}_{\Theta^{DGN}}(x) \in \mathbb{R}^{d_{net}}$

	DNPFL			FNPF
Weight	$\dot{\Theta}^{\text{V}}_t$	$=$	$-\sum_{s=1}^n \psi^{\text{V}}_{x,\Theta^{\text{DGN}}_t} e_t(s)$, $\dot{\Theta}^{\text{F}}_t = -\sum_{s=1}^n \psi^{\text{F}}_{x,\Theta^{\text{DGN}}_t} e_t(s)$	$\dot{\Theta}^{\text{V}}_t$ same as (DNFPL), $\dot{\Theta}^{\text{F}}_t = 0$
NPF	$\dot{\phi}_{x_s,\Theta^{\text{F}}_t}(p)$	$=$	$x(\mathcal{I}_0(p)) \sum_{\theta^{\text{F}} \in \Theta^{\text{F}}} \partial_{\theta^{\text{F}}} A_{\Theta^{\text{F}}_t}(x_s, p) \dot{\theta}^{\text{F}}_t, \forall p \in [P], s \in [n]$	$\dot{\phi}_{x_s,\Theta^{\text{F}}_t}(p) = 0$
NPV	$\dot{v}_{\Theta^{\text{V}}_t}(p)$	$=$	$\sum_{\theta^{\text{V}} \in \Theta^{\text{V}}} \partial_{\theta^{\text{V}}} v_{\Theta^{\text{V}}_t}(p) \dot{\theta}^{\text{V}}_t, \forall p \in [P]$	$\dot{v}_{\Theta^{\text{V}}_t}(p)$ same as DNPFL
Kernel	$K_{\Theta^{\text{DGN}}}$	$=$	$K^{\text{V}}_{\Theta^{\text{DGN}}} + K^{\text{F}}_{\Theta^{\text{DGN}}}$	$K_{\Theta^{\text{DGN}}} = K^{\text{V}}_{\Theta^{\text{DGN}}}$
Error	$\dot{e}_t$	$=$	$-\left(K_{\Theta^{\text{DGN}}_t}\right) e_t$	$\dot{e}_t = -\left(K_{\Theta^{\text{DGN}}_t}\right) e_t$

• The gradient dynamics in a DGN specified in Proposition 4.1 is similar to the gradient dynamics in a DNN specified in Proposition 3.4. Important difference is that in a DGN there are $2d_{net}$ parameters, that value gradient $\psi^{\text{V}}_{x,\Theta^{\text{DGN}}}$ flows through the value network and the feature gradient $\psi^{\text{F}}_{x,\Theta^{\text{DGN}}}$ flows through the feature network. As a result $K^{\text{CROSS}}_{\Theta} = 0$. Note that in the FNPF mode of the DGN, since $\Theta^{\text{F}} \in \mathbb{R}^{d_{net}}$ are non-trainable $\psi^{\text{F}} = 0$, and hence $\dot{\phi} = 0$ and $K^{\text{F}}_{\Theta} = 0$.

5 Measure Of Gating Information and Neural Path Kernel

We now provide theoretical justification for "Claim I", i.e., the information in the gates of a DNN is captured in its active sub-networks. We define gating information as below.

Definition 5.1 (Measure of Gating Information)**.** *Define the measure of information stored in a* DNN *with parameter* $\bar{\Theta} \in \mathbb{R}^{d_{net}}$ *to be the generalisation performance of a* DGN *with identical architecture operated in the* FNPF *mode whose* $\Theta^F_0 = \bar{\Theta}$ *are non-trainable, and* $\Theta^V \in \mathbb{R}^{d_{net}}$ *are trained.*

Suppose we train a standard DNN for T epochs, and say the parameter at end of training is $\bar{\Theta}_T$. In this case, the relation learnt is $\hat{y}_{\bar{\Theta}_T} = \Phi_{\bar{\Theta}_T} v_{\bar{\Theta}_T}$. Thus, while measuring information in the gates of this trained DNN, as per Definition 5.1, we are retaining $\Phi_{\bar{\Theta}_T}$ by storing the weights as $\Theta^{\text{F}}_0 = \bar{\Theta}_T$ in the gating network, and discarding $v_{\bar{\Theta}_T}$, and re-training Θ^{V} to learn a new relation $\hat{y}_{\Theta^{\text{DGN}}} = \Phi_{\Theta^{\text{F}}_0} v_{\Theta^{\text{V}}} = \Phi_{\bar{\Theta}_T} v_{\Theta^{\text{V}}}$.

Assumption 1. *(i)* $\Theta^V_0 \in \mathbb{R}^{d_{net}}$ *is statistically independent of* Θ^F_0*, (ii)* Θ^V_0 *are sampled i.i.d from symmetric Bernoulli over* $\{-\sigma, +\sigma\}$.

Theorem 5.1. *For $4d/w^2 < 1$, as $w \to \infty$, $K_{\Theta_0^{DGN}} \to d\sigma^{2(d-1)} H_{\Theta_0^F} = d\Sigma \odot \bar{\Lambda}_{\Theta_0^F}$, where $\bar{\Lambda}_{\Theta_0^F} = \sigma^{2(d-1)} \Lambda_{\Theta_0^F}$.*

• From previous results, Arora et al. [2019], Cao and Gu [2019], if follows that as $w \to \infty$, the optimisation and generalisation properties of the fixed NPF learner can be tied down to $K_{\Theta_0^{\text{DGN}}}$ and hence $H_{\Theta_0^{\text{F}}}$ (treating $d\sigma^{2(d-1)}$ as a scaling factor). "Claim I" is justified by noting that the NPK can be written as a *Hadamard* product of the input data Gram matrix and a correlation matrix of active sub-networks.

• In our experiments we choose $\sigma = \frac{2}{w}$. Informally speaking, for symmetric randomised initialisation of Θ_0^{F}, we expect $\frac{w}{2}$ gates to be on every layer, so $\sigma = \frac{2}{w}$ is a normalising choice, because, the diagonal entries of $\bar{\Lambda}_{\Theta_0^{\text{F}}}(s,s) \approx 1$ in this case.

• We discuss a more detailed version of Theorem 5.1 in the Appendix, where we discuss the role of width and depth on a pure memorisation task.

6 Experiments

In this section, we experimentally verify "Claim II", that is, dynamics of the gates is key for generalisation. We compare the performance of the following networks on standard MNIST and CIFAR-10 datasets: i) fixed random (FRNPF): in the DGN, we randomly initialise both $\Theta_0^{\text{F}}, \Theta_0^{\text{V}}$, make Θ^{F} *non-trainable* and train only Θ^{V} , ii) fixed learnt (FLNPF): we initialise Θ_0^{V} randomly, and copy weights from a pre-trained ReLU network (of identical architecture) into Θ_0^{F}. Similar to FR case, Θ^{F} is non-trainable and only Θ^{V} is trained iii) decoupled earning (DNPFL): we randomly initialise both $\Theta_0^{\text{F}}, \Theta_0^{\text{V}}$, and train both Θ^{F} and Θ^{V}, iv) Standard ReLU (ReLU). The results of our experiments on CIFAR-10 (please look at the Table 2 for complete results in CIFAR-10 as well as MNIST) that supports "Claim II' can be summarised as below:

1. FRNPF trains and generalises (67.08%), but ReLU (80.43%) and DNPFL (77.12%) perform better. This clearly shows that dynamics in the gates is key for generalisation.

2. FLNPF with weights copied from a fully trained ReLU performs close to 79.68% which is almost as good as ReLU (80.43%). Since from Theorem 5.1 we know that the generalisation performance of the fixed NPF learner is characterised by its NPK, and the fact that FLNPF almost recovers the performance of ReLU, we observe that *almost all the information learnt by a standard ReLU DNN is stored in its gates.*

3. The NPFs are learnt continuously during the training, and the performance gap between FRNPF and ReLU is continuous. We trained a DNN with ReLU (parameterised by $\bar{\Theta}$) for 60 epochs, and we obtained 6 different weights at various *stages* of the training process. Stage 1: $\bar{\Theta}_{10}$, stage 2: $\bar{\Theta}_{20}$, stage 3: $\bar{\Theta}_{30}$, stage 4: $\bar{\Theta}_{40}$, stage 5: $\bar{\Theta}_{50}$, stage 6: $\bar{\Theta}_{60}$. We copy these weights obtained at various stages of training to setup 6 different FLNPFs, i.e., FLNPF-1 to FLNPF-6. We observe that the performance of FLNPF-1 to FLNPF-6 increases monotonically, with FLNPF-1 performing 72% which is better than FRNPF (i.e., 67.08%), and FLNPF-6 performing as well as ReLU (see Figure 2). The performance of the Convolutional NTK based pure kernel method in Arora et al. [2019] is 77.43%. Thus through its various stages, the FLNPF starts from below 77.43% and surpasses to reach 79.68%, which implies the difference in performance is clearly coming from learning of NPFs.

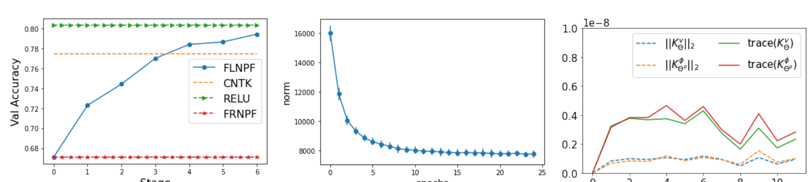

Figure 2: Dynamics of Learning

NPK during training: We considered "Binary"-MNIST data set with two classes namely digits 4 and 7, with the labels taking values in $\{-1, +1\}$ and squared loss. We trained a standard DNN with ReLU activation ($w = 100$, $d = 5$). Let $\widehat{H}_t = \frac{1}{trace(H_t)} H_t$ be the normalised NPK matrix. For a

Arch	Optimiser	Dataset	FRNPF (II)	FRNPF (DI)	DNPFL	FLNPF	ReLU
FC	SGD	MNIST	95.85 ± 0.10	95.85 ± 0.17	97.86 ± 0.11	97.10 ± 0.09	97.85 ± 0.09
FC	Adam	MNIST	96.02 ± 0.13	96.09 ± 0.12	$\mathbf{98.22 \pm 0.05}$	$\mathbf{97.82 \pm 0.02}$	$\mathbf{98.14 \pm 0.07}$
VCONV	SGD	CIFAR-10	58.92 ± 0.62	58.83 ± 0.27	63.21 ± 0.07	63.06 ± 0.73	67.02 ± 0.43
VCONV	Adam	CIFAR-10	64.86 ± 1.18	64.68 ± 0.84	$\mathbf{69.45 \pm 0.76}$	$\mathbf{71.4 \pm 0.47}$	$\mathbf{72.43 \pm 0.54}$
GCONV	SGD	CIFAR-10	67.36 ± 0.56	66.86 ± 0.44	$\mathbf{74.57 \pm 0.43}$	$\mathbf{78.52 \pm 0.39}$	$\mathbf{78.90 \pm 0.37}$
GCONV	Adam	CIFAR-10	67.09 ± 0.58	67.08 ± 0.27	$\mathbf{77.12 \pm 0.19}$	$\mathbf{79.68 \pm 0.32}$	$\mathbf{80.43 \pm 0.35}$

Table 2: Shows the training and generalisation performance of various NPFs.

subset size, $n' = 200$ (100 examples per class) we plot $\nu_t = y^\top(\widehat{H}_t)^{-1}y$, (where $y \in \{-1, 1\}^{200}$ is the labelling function), and observe that ν_t reduces as training proceeds (see middle plot in Figure 2). Note that, $\nu_t = \sum_{i=1}^{n'}(u_{i,t}^\top y)^2(\hat{\rho}_{i,t})^{-1}$, where $u_{i,t} \in \mathbb{R}^{n'}$ are the orthonormal eigenvectors of $\widehat{H}_t$ and $\hat{\rho}_{i,t}, i \in [n']$ are the corresponding eigenvalues. Since $\sum_{i=1}^{n'} \hat{\rho}_{i,t} = 1$, the only way ν_t reduces is when more and more energy gets concentrated on $\hat{\rho}_{i,t}$s for which $(u_{i,t}^\top y)^2$s are also high.

Role of K_Θ^{V} and K_Θ^{F}: In this case the of decoupled learning, NTK is given by $K_{\Theta^{\text{DGN}}} = K_{\Theta^{\text{DGN}}}^{\text{V}} + K_{\Theta^{\text{DGN}}}^{\text{F}}$. For MNIST, we compared $K_{\Theta^{\text{DGN}}}^{\text{V}}$ and $K_{\Theta^{\text{DGN}}}^{\text{F}}$ using their trace and Frobenius norms, and we observe that K_Θ^v and $K_{\Theta^{\text{F}}}^\phi$ are in the same scale, which is perhaps pointing to the fact that both K_Θ^v and $K_{\Theta^{\text{F}}}^\phi$ are equally important for obtaining good generalisation performance.

6.1 Experimental Setup

We used standard datasets namely MNIST and CIFAR-10, with categorical cross entropy loss. We used stochastic gradient descent (SGD) and *Adam*. In the case of SGD, we tried constant step-sizes in the set $\{0.1, 0.01, 0.001\}$ and chose the best. In the case of Adam the we used a constant step size of $3e^{-4}$. In both cases, we used batch size to be 32. We used a fully connected (FC) DNN with $(w = 128, d = 6)$ for MNIST. To train CIFAR-10, we used *Vanilla-Convolutional* Network (VCONV) without pooling, residual connections, dropout or batch-normalisations, and is given by: input layer is $(32, 32, 3)$, followed by convolution layers with a stride of $(3, 3)$ and channels 64, 64, 128, 128 followed by a flattening to layer with 256 hidden units, followed by a fully connected layer with 256 units, and finally a 10 width soft-max layer to produce the final predictions. To train CIFAR-10, we also used a GCONV which is same as VCONV with a *global-average-pooling* (GAP) layer. For both FRNPF, and FLNPF, we let $\chi^{\text{F}} = \chi_r$, and $G_{x,t}(l) = \gamma_r\left(q_{x,t}^{\text{F}}(l)\right)$. In the case of FRNPF, we considered two possible initialisations namely i) *independent initialisation* (II), i.e., Θ_0^{F} and Θ_0 are statistically independent, and ii) *dependent initialisation* (DI), i.e., $\Theta_0^{\text{F}} = \Theta_0$, a case which mimics the NPFs and NPVs of a standard DNN with ReLU activations. In the case of FLNPF, $\Theta_0^{\text{F}} = \bar{\Theta}$, where $\bar{\Theta}$ is the parameter of a pre-trained (could be in various stages of training) DNN with ReLU activations. In the case, DNPFL, we let $\chi^{\text{F}} = \chi_r$, and $G_{x,t}(l) = \gamma_{sr}\left(q_{x,t}^{\text{F}}(l)\right)$ with $\beta = 8$. The use of soft-ReLU makes it straightforward for the feature gradients to flow via the gating network.

7 Conclusion and Future Work

Gradient is a first-order information, and learning with GD is essentially a process of integration, and naturally its outcome is a zeroth-order information. It turns out the NPFs capture this zeroth-order information, and plays a critical role in DNNs. We conclude by saying:

Understanding deep learning requires understanding the dynamics of the neural path features.

A possible future direction is to understand the role of depth and width in NPF learning, and the role of NPF in generalisation. The deep gated network might be useful in this effort, since the NPFs learning is decoupled and is perhaps easier to analysis than standard DNNs.

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